Mathematical Biosciences and Engineering

MBE, 18(3): 2372–2383.
DOI: 10.3934/mbe.2021120
Received: 30 January 2021
Accepted: 05 March 2021
Published: 09 March 2021

http://www.aimspress.com/journal/MBE

Research article

Electrostatic features for nucleocapsid proteins of SARS-CoV and SARS-CoV-2

Wenhan Guo[1], Yixin Xie[1], Alan E Lopez-Hernandez[1], Shengjie Sun[1] and Lin Li[1,2,*]

[1] Computational Science Program, University of Texas at El Paso, El Paso, TX 79968, USA
[2] Department of Physics, University of Texas at El Paso, El Paso, TX 79968, USA

* **Correspondence:** Email: lli5@utep.edu.

Abstract: COVID-19 is increasingly affecting human health and global economy. Understanding the fundamental mechanisms of Severe Acute Respiratory Syndrome CoronaVirus 2 (SARS-CoV-2) is highly demanded to develop treatments for COVID-19. SARS-CoV and SARS-CoV-2 share 92.06% identity in their N protein RBDs' sequences, which results in very similar structures. However, the SARS-CoV-2 is more easily to spread. Utilizing multi-scale computational approaches, this work studied the fundamental mechanisms of the nucleocapsid (N) proteins of SARS-CoV and SARS-CoV-2, including their stabilities and binding strengths with RNAs at different pH values. Electrostatic potential on the surfaces of N proteins show that both the N proteins of SARS-CoV and SARS-CoV-2 have dominantly positive potential to attract RNAs. The binding forces between SARS-CoV N protein and RNAs at different distances are similar to that of SARS-CoV-2, both in directions and magnitudes. The electric filed lines between N proteins and RNAs are also similar for both SARS-CoV and SARS-CoV-2. The folding energy and binding energy dependence on pH revealed that the best environment for N proteins to perform their functions with RNAs is the weak acidic environment.

Keywords: SARS-CoV; SARS-CoV-2; COVID-19; protein-protein interactions; protein-RNA/DNA interactions; electrostatic force; DelPhi; DelPhiForce

Supplementary

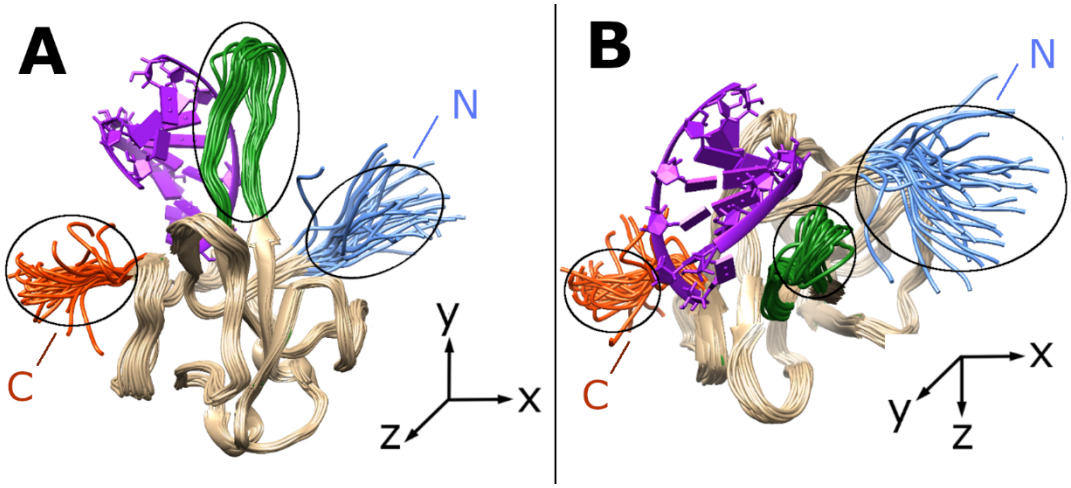

Figure S1. (A) The side view of the structure of SARS-CoV-2 N protein RBD bind with RNA; (B) The top view of the structure of SARS-CoV-2 N protein RBD bind with RNA. The N terminals are shown with blue color while the C terminals are displayed with orange color. The flexible hairpin-like structures of SARS-CoV-2 N protein RBDs are highlighted with green color.